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MOLECULAR AND MASS SPECTROSCOPIC ANALYSIS OF ISOTOPICALLY
LABELED ORGANIC RESIDUES^a.

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INTRODUCTION

Experimental studies aimed at understanding the evolution of complex organic molecules on interstellar grains have been performed.

The photolysis of frozen gas mixtures of various composition containing H₂O; CO; NH₃ and CH₄ was studied. These species were chosen because of their astrophysical importance as deduced from observational as well as theoretical studies of ice mantles on interstellar grains.

These ultraviolet photolysed ices were warmed up in order to produce refractory organic molecules like the ones formed in molecular clouds when the icy mantles are being irradiated and warmed up either by a nearby stellar source or impulsive heating.

The laboratory studies give us among other results, estimates of the efficiency of production of such organic material under interstellar conditions. There is sufficient production of organic material in molecular clouds (Schutte, 1988) to maintain organic refractory mantles against the destructive processes in diffuse clouds (Greenberg, 1982 and 1986).

RESULTS

ANALYSIS OF ORGANIC RESIDUES (O.R.)Non-isotopically labeled samples.

The O.R. was analysed by GC-MS and HPLC. Previous studies (Agarwal et al, 1985 and Schutte, 1988) showed that the O.R. consists of a number of small molecules containing hydroxy, carbonyl and amine-groups. In table 1 a summary of the photoproducts from different ratios of the mixture H₂O:CO:NH₃:CH₄ is shown.

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TABLE 1. Molecular composition of O.R. made from the gas mixture H₂O: CO: NH₃: CH₄ in the following ratios:
 Sample one: 5:5:1:0, sample two: 3: 1: 0.3: 1 and sample three: 8: 0: 1: 2.5.
 (from Agarwal et al 1985, Ferris 1987 and Schutte 1988).

PHOTOPRODUCTS		SAMPLE NR.		
Name	Formulae	1	2	3
		Abundances		
Glycolic Acid	HOCH ₂ COOH	0.50	0.38	0.21
3-Hydroxypropanoic acid	HOCH ₂ CH ₂ COOH	(*)	(*)	0.06
Formamidine	HN=CHNH ₂	-	-	0.20
Hydroxy-acetamide	HOCH ₂ CONH ₂	0.18	0.13	0.11
Hexamethylene-Tetramine	C ₆ H ₁₂ N ₄	(*)	(*)	0.13
Urea/Biuret (**)	H ₂ NCONH ₂ / H ₂ NCONHCONH ₂	0.01	-	-
Oxamic acid	H ₂ NCOCOOH	0.02	0.05	-
Ethanol-amine	H ₂ NCH ₂ CH ₂ OH	0.006	-	0.10
Glycerol	HOCH ₂ CHOHCH ₂ OH	0.04	0.06	0.06
Glycine	H ₂ NCH ₂ COOH	-	-	0.02
Oxamide	H ₂ NCOCONH ₂	0.07	0.15	0.06
Glyceric acid	HOCH ₂ CHOHCOOH	0.06	0.07	0.05
Glyceramide	HOCH ₂ CHOHCONH ₂	0.12	0.16	0.002

Notes:

(*) Detected, but amount not measured

(**) Urea and biuret analyzed together

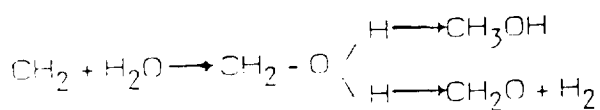
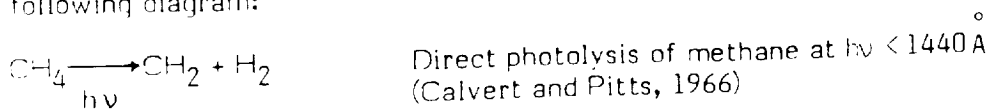
Isotopically labeled samples.

Because of being able to prepare only very small samples in the laboratory, there are always problems of contamination to be worried about. Therefore one has to be cautious of all sources of contamination, not only leaks in the system, but also residual deposits left over from earlier experiments in the apparatus.

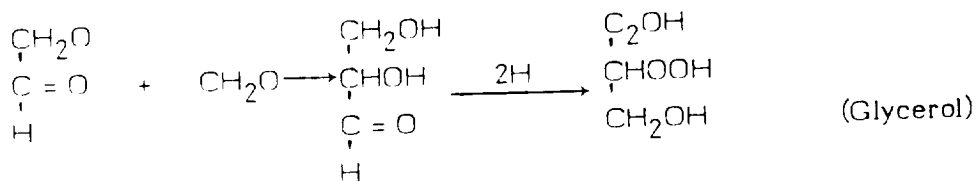
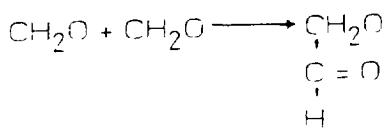
In order to detect contamination and to better identify the molecules, we started on a new program using isotopically labeled mixtures. One first result

was that glycerol, one of the less abundant products - and thus with more possibilities of having come from contamination - has been clearly identified in the residues with isotopic labelling.

A proposed scheme for the process leading to glycerol is shown in the following diagram:



obtaining thus formaldehyde (CH_2O). Then,



CONCLUSIONS

Our ultimate aim is to understand the evolution of mantles of interstellar grains and to account for both their chemical and physical properties - including their optical properties from the submillimeter to the ultraviolet.

The gradual carbonization of organic mantles in the diffuse cloud phase leads to higher and higher visual absorptivity - yellow residues become brown in the laboratory.

Our results are being applied to explaining the organic components of comets and their relevance to the origin of life.

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